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Calculation of Collision Cross Sections with CTMC Codes

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The Classical Trajectory Monte Carlo (CTMC) method has been used successfully in cross section calculations in various cases of collisions involving electrons, atoms, ions and molecules [1]. Besides being designed to calculate these cross sections, the CTMC method is of interest in the study of chaotic systems [2]. The various versions of the application codes differ mainly in the number of bodies taken into account (currently three-, four- and five-body problems), the potential allowed for the bodies (of which the Coulomb potential is the most evident choice) and the treatment of the distribution function(s), initially a purely micro-canonical one.
We report here recent work calculations of CTMC collision cross sections of interest to thermonuclear fusion. One aspect of the work involves ion ion collision cross sections at energies from approximately one keV/u up to several MeV/u. Collisions of metallic and of Ne ions with hydrogen atoms were previously studied using this CTMC code [3]. This work is now extended to the study of collisions of rare gas species in various ionization stages. Parametric potentials [4] are used throughout for the collision centers.
Another class of CTMC calculations in progress involves somewhat lower energy collisions of neutral sodium atoms constituting a neutral beam, colliding with low Z atoms and ions. As was the case with previous calculations involving He atoms [5], use of Coulomb potentials is expected to be sufficient in this case.
The CTMC method has the advantage of allowing the calculation of ionization and charge transfer cross sections simultaneously. The problem of excitation evaluation is more complicated, due to the large number of possible exit channels. However, the method has been used in cases where only a small number of excitation channels are important [6].
Calculated results for these two cases will be presented and discussed during the Conference.

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